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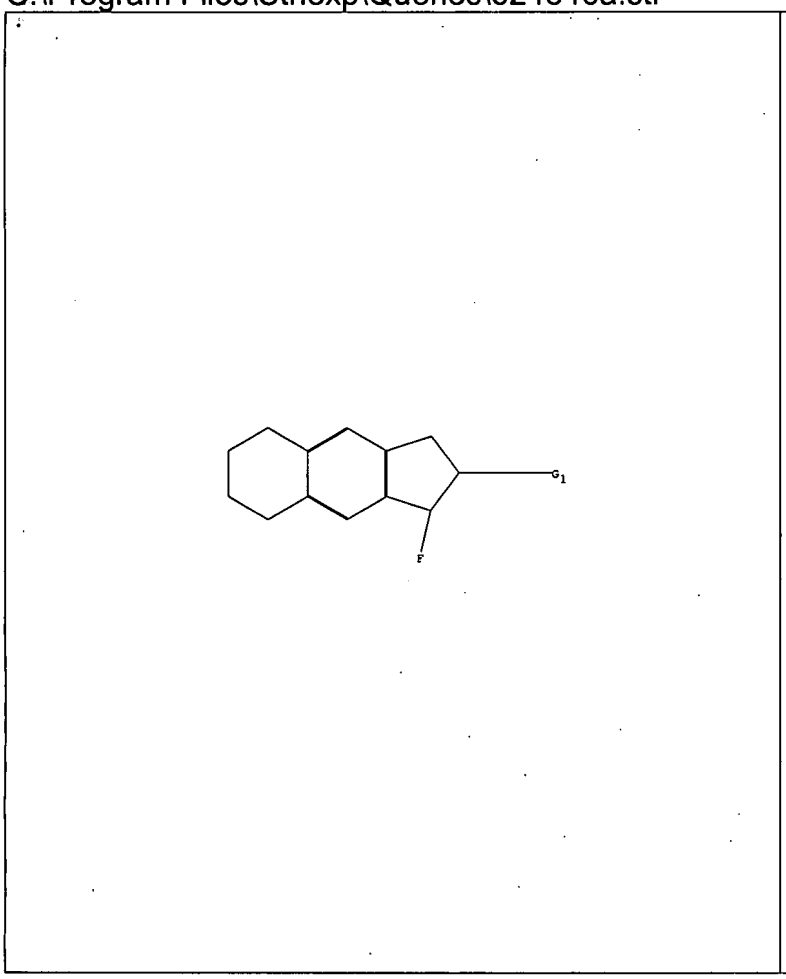

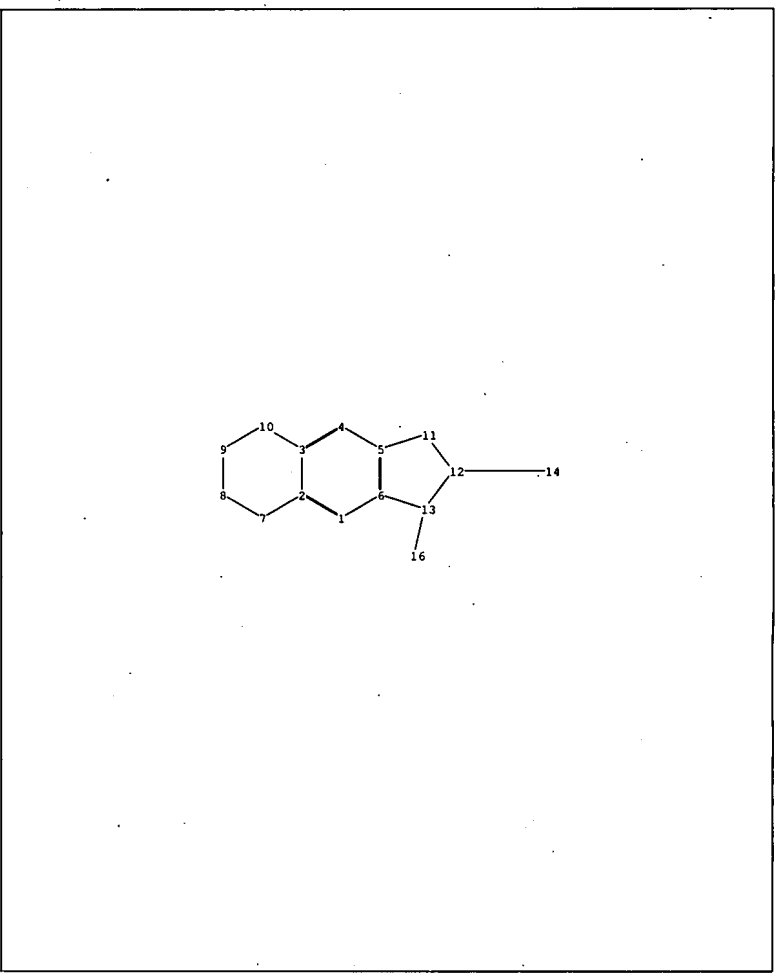

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14 16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
12-14 13-16
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 5-11 6-13 7-8 8-9 9-10 11-12 12-13
exact/norm bonds :
2-7 3-10 5-11 6-13 7-8 8-9 9-10 11-12 12-13 12-14
exact bonds :
13-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 16:CLASS

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:203786 CAPLUS
DN 140:243724
ED Entered STN: 14 Mar 2004
TI Cyclopenta[b]naphthalene derivatives
IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie; Heckmeier, Michael
PA Merck Patent G.m.b.H., Germany
SO PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07C025-22
ICS C07C022-08; C07C025-24; C07C043-225; C09K019-32
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75
FAN.CNT 2

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PI	WO 2004020375	A1	20040311	WO 2003-EP8285	20030728
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	EP 1532090	A1	20050525	EP 2003-790821	20030728
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005537334	T	20051208	JP 2004-569707	20030728
	US 2006165915	A1	20060727	US 2005-524846	20050218
PRAI	DE 2002-10238999	A	20020826		
	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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	IPCI	C07C0025-22 [ICM,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]
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		[ICS,7,C*]; C07C0025-00 [ICS,7]; C07C0025-24 [ICS,7]
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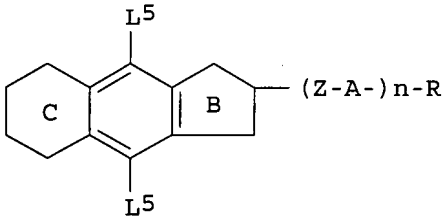
	NCL	428/001.100; 252/299.610; 252/299.620; 585/021.000
	ECLA	C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24; C07C017/35+25/22; C07C017/35+25/24; C07C017/354+25/22; C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697; C07C045/46+49/755; C07C045/64+49/747; C07C049/697; C07C255/52; C09K019/32; C09K019/34A

OS MARPAT 140:243724

GI



I

AB The invention relates to cyclopenta[b]naphthalene derivs. of general formula I (C =6-membered ring with substituents selected from H, C1-15-alkyl, alkoxy, etc.; B = 5-membered ring with substituents selected from H, C1-15-alkyl, alkoxy, etc.; Z = single bond, double bond, -CF2O-, -OCF2-, etc.; A = 1,4-phenylene, 1,4-cyclohexylene, etc.; R = H, C1-15-alkyl, alkoxy, etc.; L5, L6 = H, C1-15-alkyl, alkoxy, etc.; n = 0-3), the use thereof in liquid crystal or mesogenous media, liquid crystal or mesogenous media comprising at least one of said cyclopenta[b]naphthalene

derivs. and electrooptical display elements comprising said liquid crystal or mesogenous media.

ST cyclopenta naphthalene synthesis liq crystal mesogenous media electrooptical display

IT Liquid crystal displays
Liquid crystals
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P
666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P
666732-99-6P 666733-01-3P 666733-03-5P 666733-05-7P 666733-07-9P
666733-09-1P 666733-11-5P 666733-13-7P
666733-15-9P 669005-43-0P 669005-44-1P 669005-45-2P
669005-46-3P 669005-47-4P 669005-48-5P 669005-49-6P 669005-50-9P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 75-77-4, Chlorotrimethylsilane, reactions 100-39-0, Benzylbromide
540-63-6, 1,2-Ethanedithiol 7664-39-3, Hydrofluoric acid, reactions
7719-09-7, Thionylchloride 57848-46-1 64248-58-4 104089-16-9
107263-95-6, N-Fluoropyridinium triflate 610312-65-7 669005-29-2
669005-36-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 13772-59-3P 666732-11-2P 666732-13-4P 666732-15-6P 666732-17-8P
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666732-57-6P 666732-59-8P 666732-61-2P 666732-63-4P 666732-65-6P
666732-67-8P 666732-69-0P 666732-71-4P 666732-74-7P 666732-76-9P
666732-79-2P 666732-81-6P 666732-83-8P 669005-26-9P 669005-27-0P
669005-28-1P 669005-30-5P 669005-31-6P 669005-32-7P 669005-33-8P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 669005-40-7P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Clariant International; EP 1223209 A 2002 CAPLUS
(2) Hoechst Ag; DE 4434974 A 1996 CAPLUS
(3) Merck Patent Gmbh; WO 0246330 A 2002 CAPLUS
(4) Montell Technology Co; WO 9846547 A 1998 CAPLUS
(5) Yokokoji, O; JP 06263663 A 1994 CAPLUS

IT 666732-85-0P 666732-87-2P 666732-89-4P
666732-91-8P 666733-11-5P 666733-13-7P
666733-15-9P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

RN 666732-85-0 CAPLUS

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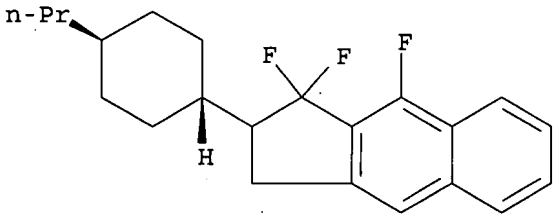
Relative stereochemistry.



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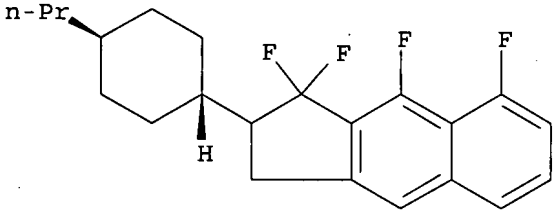
Relative stereochemistry.



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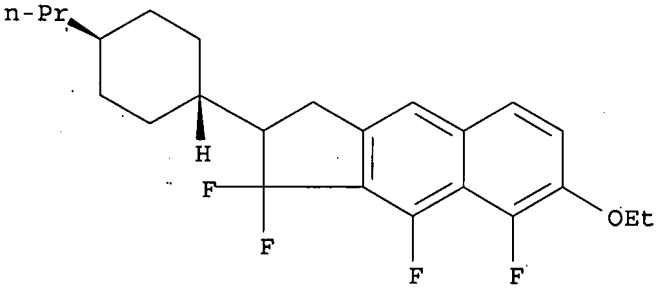
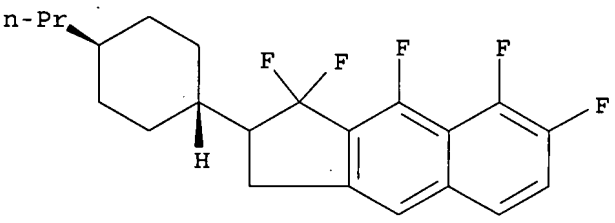
Relative stereochemistry.



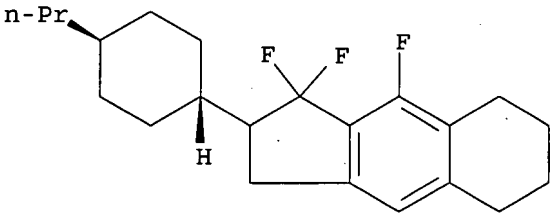
RN 666732-91-8 CAPLUS
CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 666733-11-5 CAPLUS
CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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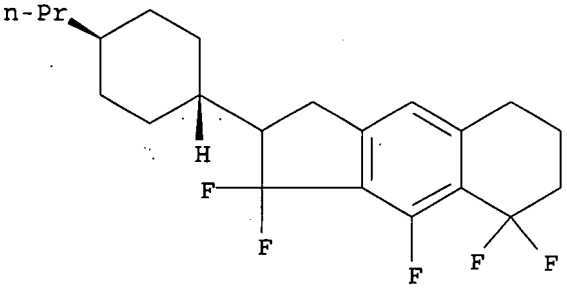
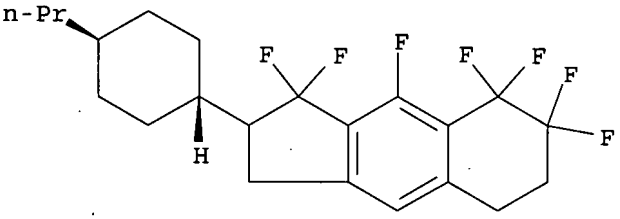
Relative stereochemistry.



RN 666733-15-9 CAPLUS
CN 1H-Benz[f]indene, 1,1,7,7,8,8,9-heptafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:177941 CAPLUS
DN 140:225895
ED Entered STN: 04 Mar 2004
TI Cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display
IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 46 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07C025-22
ICS C07C043-225; C07C049-697; C07D319-06; C09K019-32; C09K019-34; G02F001-137; G09F009-35; C07C069-00; C07C323-00; C07C255-00; C07C331-00
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other

Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10238999	A1	20040304	DE 2002-10238999	20020826
	WO 2004020375	A1	20040311	WO 2003-EP8285	20030728
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	AU 2003258538	A1	20040319	AU 2003-258538	20030728
	EP 1532090	A1	20050525	EP 2003-790821	20030728
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	JP 2005537334	T	20051208	JP 2004-569707	20030728
	US 2006165915	A1	20060727	US 2005-524846	20050218
PRAI	DE 2002-10238999	A	20020826		
	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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		C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,C*]; C09K0019-32 [I,A]; C09K0019-34 [I,C*]; C09K0019-34 [I,A]; C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13 [I,C*]; G02F0001-13 [I,A]
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AU 2003258538	IPCI	C07C0025-22 [ICM,7]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]
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	NCL	428/001.100; 252/299.610; 252/299.620; 585/021.000
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C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697;
C07C045/46+49/755; C07C045/64+49/747; C07C049/697;
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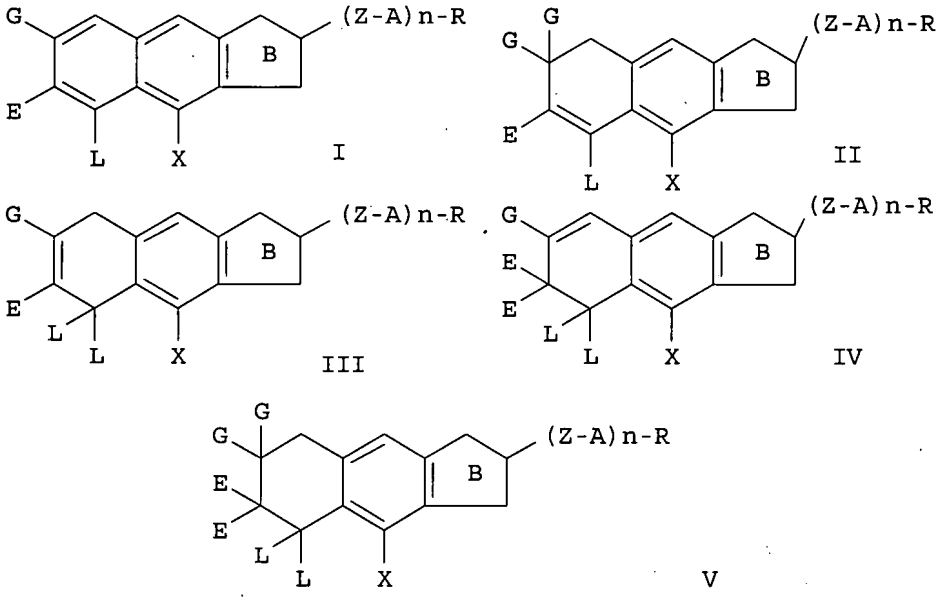
OS MARPAT 140:225895

GI



AB The title cyclopenta[b]naphthalene derivative having a neg. Δε is represented by general formula I, II, III, IV and V (B = five membered ring with F-substituent; A = 1,4-phenylene, etc.; Z = single bond, double bond, -CF2O-, etc.; R = H, C1-15-alkyl, alkoxy, etc.; X, L = H, C1-15-alkyl, etc.; E, G = H, C1-15-alkyl, etc.; n = 0-3). The cyclopenta[b]naphthalene derivs. are synthesized.

ST nematic liq crystal mixt display cyclopenta naphthalene prepn

IT Liquid crystal displays
(cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT Liquid crystals
(nematic; cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P
666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P
666732-99-6P 666733-01-3P 666733-03-5P 666733-05-7P 666733-07-9P
666733-09-1P 666733-11-5P 666733-13-7P
666733-15-9P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 75-77-4, Chlorotrimethylsilane, reactions 77-48-5, 1,3-Dibromo-5,5-dimethylhydantoin 100-39-0 109-80-8, 1,3-Propanedithiol 540-63-6, 1,2-Ethanedithiol 7664-39-3, Hydrogen fluoride, reactions 57848-46-1 104089-16-9 107263-95-6, N-Fluoropyridinium triflate 610312-65-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

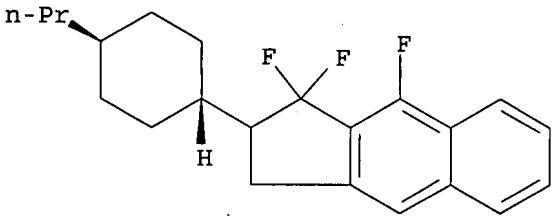
IT 13772-59-3P 666732-11-2P 666732-13-4P 666732-15-6P 666732-17-8P
666732-19-0P 666732-22-5P 666732-24-7P 666732-26-9P 666732-28-1P

666732-30-5P 666732-32-7P 666732-36-1P 666732-38-3P 666732-40-7P
666732-42-9P 666732-44-1P 666732-46-3P 666732-48-5P 666732-50-9P
666732-52-1P 666732-55-4P 666732-57-6P 666732-59-8P 666732-61-2P
666732-63-4P 666732-65-6P 666732-67-8P 666732-69-0P 666732-71-4P
666732-74-7P 666732-76-9P 666732-79-2P 666732-81-6P 666732-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P
666732-91-8P 666733-11-5P 666733-13-7P
666733-15-9P
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

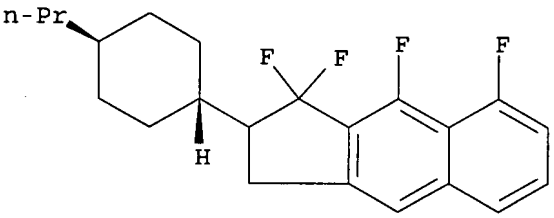
RN 666732-85-0 CAPLUS
CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



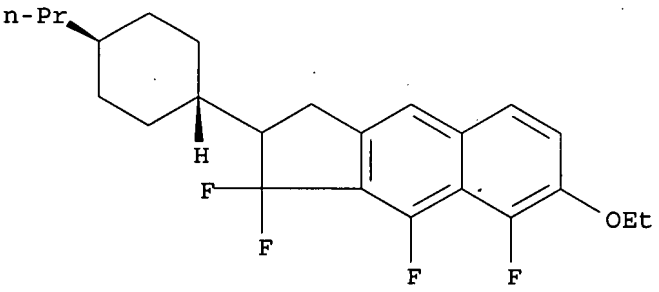
RN 666732-87-2 CAPLUS
CN 1H-Benz[f]indene, 1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



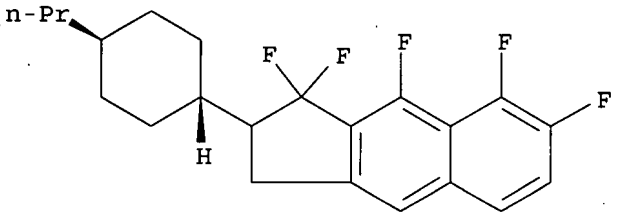
RN 666732-89-4 CAPLUS
CN 1H-Benz[f]indene, 7-ethoxy-1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 666732-91-8 CAPLUS
CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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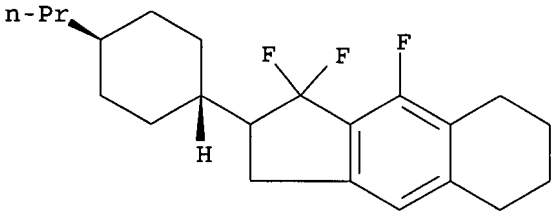
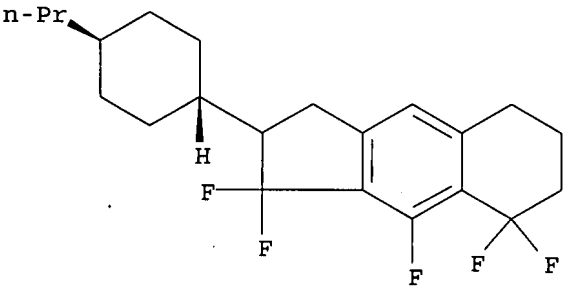
CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



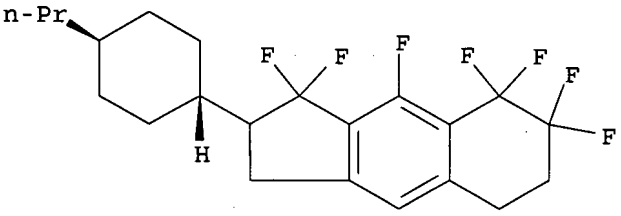
RN 666733-13-7 CAPLUS
CN 1H-Benz[f]indene, 1,1,8,8,9-pentafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 666733-15-9 CAPLUS
CN 1H-Benz[f]indene, 1,1,7,7,8,8,9-heptafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:817619 CAPLUS
DN 138:237618
ED Entered STN: 28 Oct 2002
TI MNDO Study of the (Anti)aromaticity of Fluorine-Containing Cyclopentadienyl, Indenyl, and Cyclopenta[b]naphthyl Cations
AU Shchegoleva, L. N.; Karpov, V. M.; Platonov, V. E.
CS Siberian Division, Vorozhtsov Novosibirsk Institute of Organic Chemistry, Russian Academy of Sciences, Novosibirsk, 630090, Russia
SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2002), 38(7), 995-1000
CODEN: RJOCEQ; ISSN: 1070-4280
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA English
CC 22-2 (Physical Organic Chemistry)
AB MNDO calcns. were performed to estimate the aromaticity (antiaromaticity) of F-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations in terms of the Dewar-Breslow criterion which uses the difference in the enthalpies of formation of isomeric cations with closed and open π-systems as aromaticity index. The aromaticity is strongly determined by both the structure of the C skeleton and the number and position of F atoms. A linear correlation was revealed between the aromaticity index and the energy of the lowest singlet-singlet excitation for cations having a cyclic π-system.
ST MNDO aromaticity antiaromaticity fluorine cyclopentadienyl indenyl cyclopentanaphthyl cation
IT Linear free energy relationship
(Dewar-Breslow aromaticity index vs. singlet excitation; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
IT Antiaromaticity
Aromaticity
Correlation analysis
Formation enthalpy
Frontier molecular orbital
HOMO (molecular orbital)
Jahn-Teller effect
LUMO (molecular orbital)
MNDO
Singlet state excitation
Substituent effects
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
IT Carbocations
RL: PRP (Properties)
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
IT Indexes
(aromaticity; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
IT Isomers
(cation; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
IT 49762-89-2 58741-78-9 62302-99-2 128654-07-9 192275-45-9
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501370-93-0
RL: PRP (Properties)
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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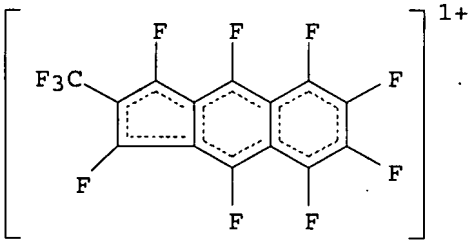
(2) Breslow, R; Acc Chem Res 1973, V6(12), P393 CAPLUS
(3) Breslow, R; Chem Eng News 1965, V43(26), P90 CAPLUS
(4) Breslow, R; Pure Appl Chem 1971, V28(2-3), P111 CAPLUS
(5) Dewar, M; The Molecular Orbital Theory of Organic Chemistry 1969
(6) Karpov, V; Russ J Org Chem 1999, V35(1), P80 CAPLUS
(7) Karpov, V; Russ J Org Chem 2001, V37(7), P981 CAPLUS
(8) Karpov, V; Tetrahedron 1978, V34(21), P3215 CAPLUS
(9) Schaftenaar, G; QCPE-619
(10) Shchegoleva, L; Zh Strukt Khim 1996, V37(6), P1023
(11) Shchegoleva, L; Zh Strukt Khim 1999, V40(1), P184
(12) Stewart, J; MOPAC 7.0
(13) Zhou, Z; J Phys Org Chem 1990, V3(12), P784 CAPLUS
IT 501370-90-7 501370-91-8
RL: PRP (Properties)
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
RN 501370-90-7 CAPLUS
CN Benz[f]indenylium, 1,3,4,5,6,7,8,9-octafluoro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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CN Benz[f]indenylium, 1,3,4,5,8,9-hexafluoro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)